FRI-1.417-1-MEMBT-05

MODELLING OF THE BOUNDARY CONDITION FOR MICRO CHANNELS WITH USING LATTICE BOLTZMANN METHOD (LBM)

Rsc. Asst. İlkay Çolpan, BSc
Department of Mechanical Engineering,
Kırklareli University, Kırklareli
E-mail: ilkaycolpan@klu.edu.tr

Asst. Prof. Erman Aslan, PhD
Department of Mechanical Engineering,
Istanbul University, Istanbul
Phone: +90 212 4737070 /17820
E-mail: erman.aslan@istanbul.edu.tr

Prof. Hasan Rıza Güven, PhD
Department of Mechanical Engineering,
Istanbul University, Istanbul
Phone: +90 212 4737070 /17824
E-mail: hrguven@istanbul.edu.tr

Abstract: *Modelling of the boundary condition for micro channels with using Lattice Boltzmann Method (LBM) are investigated numerically in this work. Poiseuille flow in the continuum, slip and transition regimes is examined by using bounce-back, reflection factor and accommodation coefficient boundary conditions on solid walls with different mesh numbers. Numerical results from Lattice Boltzmann Method (LBM) are compared with analytical results.*

Keywords: *Lattice Boltzmann Method, Micro Channel, Boundary Conditions*

INTRODUCTION

MEMS (Micro-electro-mechanical systems) have received increasing attention due to their advantages for applications such as micro-generators, micro-sensors in various fields such as medicine, home appliances etc. (Koester, D. A., Markus, K. W. & Walters, M. D., 1996). Since the development of MEMS, fluid flows in micro-devices such as micro-channels have become important study area and gas flow in micro channels are the common configuration of micro devices in biomedical applications (Ho, C. M., & Tai, Y. C., 1998). The characteristic dimension of micro channels is of order of 1 micron to 100 microns (Tang, G. H., Tao, W. Q., & He, Y. L., 2004). The Navier-Stokes (N-S) equations and the continuum hypothesis are disabled when $Kn>0.01$ for gas flows. Knudsen number is dimensionless number which equals the ratio of the mean free path (λ) to the characteristic length (H) for gas flows. There is a method to simulate micro gas flows, which is the Direct Simulation of Monte Carlo (DSMC) (Bird, G. A., 1994). The DSMC method is a particle based method. However, DSMC method has big disadvantages. DSMC method is linked with the number of molecules, therefore the computational time is very large and DSMC method needs big computer memory to store data. The other method is Lattice Boltzmann Method (LBM) (Bhatnagar, P. L., Gross, E. P. & Krook, M., 1954) which is based on Lattice Boltzmann Equation (LBE). For the relaxation time the Bhatnagar-Gross-Krook approximation (Bhatnagar, P. L., Gross, E. P. & Krook, M., 1954) in LBM is used. LBM is not linked with number of molecules so it has low computational cost and Lattice Boltzmann Equation (LBE) is valid when $Kn>0.01$, so it is a good choice to use Lattice Boltzmann Method to simulate micro channels with large Knudsen number range.

EXPOSITION

Investigation of Lattice Boltzmann Model for Micro Flow

This equation iscalled LBGK (Lattice Bhatnagar-Gross-Krook) (Qian, Y., d'Humieres, D. & Lallemand, P., 1992) model with dimensionless single relaxation time (τ) and it can be defined as

$$f_i(x + c_i\Delta t, t + \Delta t) = f_i(x,t) + \frac{[f_i^{eq}(x,t) - f_i(x,t)]}{\tau} \tag{1}$$

where $f_i^{eq}(x,t)$ is equilibrium distribution function at x lattice site, t time and i direction. In the LBM simulation two dimensional nine velocities lattice model (D2Q9) is used. The D2Q9 model is square lattice model with central particle lattice velocity equal to zero. The D2Q9 model is shown in Fig.1.

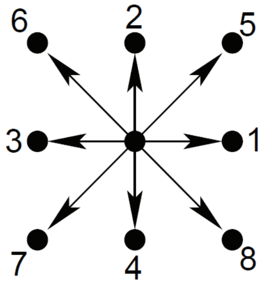

Fig. 1. D2Q9 model

And equilibrium distribution function can be written as

$$f_i^{eq} = \rho\omega_i\left[1 + \frac{3}{{c_k}^2}(c_i u) + \frac{9}{{c_k}^4}(c_i u)^2 - \frac{3}{2{c_k}^2}(u^2)\right] \tag{2}$$

where c_k speed of sound, c_i is particle velocities and ω_i is weighting factor. In micro channels Knudsen number is important parameter to determine the mean free path on gas flows. The Knudsen number can be written as

$$Kn = \frac{\lambda}{H} \tag{3}$$

where λ is mean free path of molecules and H is channel height. Knudsen number can be redefined as

$$Kn = \frac{A(\tau - 0.5)}{\rho H} \tag{4}$$

where A is constant and $A = 0.388$. In this study τ is changed with τ'.

$$\tau' = 0.5 + \frac{\tau - 0.5}{\rho} \tag{5}$$

There is a quite large density difference between inlet and outlet of the micro channel. Therefore it is important to include density on relaxation time (τ'). (Nie, X., Doolen, G.D. & Chen, S., 2002) Kinematic viscosity can be defined as

$$\vartheta = \left(\frac{\tau - 0.5}{\rho}\right) c_k^2 \Delta t \tag{6}$$

Investigation of Boundary Conditions in Micro Channels

In Fig. 2 physical boundaries with D2Q9 model in micro channel is defined. Pressure is given at inlet and outlet of micro channel to provide certain pressure ratios (1.5, 2, 2.5).

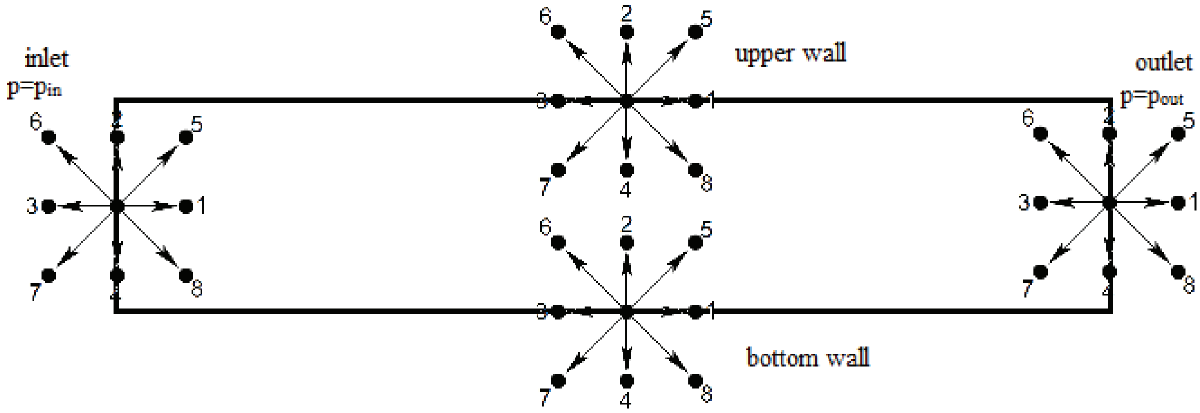

Fig. 2. D2Q9 model in a micro channel

In this study three different boundary conditions are used to simulate micro channels which are bounce-back boundary condition, accommodation coefficient boundary condition and reflection factor boundary condition. The bounce-back boundary condition for bottom wall can be written as

$$\begin{aligned} f_2(x,y,t) &= f_4(x,y+\Delta y,t-\Delta t) \\ f_5(x,y,t) &= f_7(x+\Delta x,y+\Delta y,t-\Delta t) \\ f_6(x,y,t) &= f_8(x-\Delta x,y+\Delta y,t-\Delta t) \end{aligned} \tag{7}$$

The accommodation coefficient boundary condition for bottom wall can be written as

$$\begin{aligned} f_2(x,y,t) &= a_c f_7(x+\Delta x,y+\Delta y,t-\Delta t) + a_c f_8(x-\Delta x,y \\ &\quad +\Delta y,t-\Delta t) + f_4(x,y+\Delta y,t-\Delta t) \\ f_5(x,y,t) &= (1-a_c) f_8(x-\Delta x,y+\Delta y,t-\Delta t) \\ f_6(x,y,t) &= (1-a_c) f_7(x+\Delta x,y+\Delta y,t-\Delta t) \end{aligned} \tag{8}$$

where a_c is accommodation coefficient, if a_c equals 1 then it is diffuse reflection boundary condition and if a_c equals 0 then it is specular reflection boundary condition. For upper and bottom wall the value of a_c is taken respectively 0.1, 0.6, 0.7, 0.8, 0.9, 0.99 respectively. The reflection factor boundary condition for bottom wall can be written as

$$\begin{aligned} f_2(x,y,t) &= f_4(x,y+\Delta y,t-\Delta t) \\ f_5(x,y,t) &= r_f f_7(x+\Delta x,y+\Delta y,t-\Delta t) + (1-r_f) f_8(x-\Delta x,y+\Delta y,t-\Delta t) \\ f_6(x,y,t) &= r_f f_8(x-\Delta x,y+\Delta y,t-\Delta t) + (1-r_f) f_7(x+\Delta x,y+\Delta y,t-\Delta t) \end{aligned} \tag{9}$$

where r_f is reflection factor and if $r_f = 1$ then it is no-slip boundary condition, if $r_f = 0$ then it is free-slip boundary condition. The values of reflection factor are taken for bottom and upper wall 0.1, 0.6, 0.7, 0.8, 0.85, 0.9 values.

Analytical Equations for Micro Channels

Arkilic et al. (Arkilic, E.B., Schmidt, M.A. & Breuer, K.S., 1997) obtained analytical results for slip flow in two-dimensional micro channels. One of these analytical results is pressure. The analytical equation of the pressure distribution is as follows

$$P^* = -6\sigma Kn + \sqrt{(-6\sigma Kn)^2 + (1+12\sigma Kn)X + (Pr^2 + 12\sigma Kn Pr)(1-X)} \tag{10}$$

 Copyrights© 2017 ISBN 978-954-712-733-3 (Print)

where P^* is the normalized pressure distribution. And Pr is the ratio of the pressures at the inlet and outlet of the micro channel. And Pr can be written as

$$Pr = \frac{P_{in}}{P_{out}} \tag{11}$$

where P_{in} and P_{out} are respectively inlet pressure and outlet pressure. σ is the accommodation factor and it equals 1. X is the normalized position. X is obtained by dividing the lattice position by the length of the microchannel

$$X = \frac{x}{L} \tag{12}$$

Where L is the length of micro channel. In order to find non-linearity of pressure, it is necessary to find linear pressure distribution (P_{linear}).

$$P_{linear} = P_{out} + (P_{in} - P_{out})(1 - X) \tag{13}$$

$$P' = P^* - P^*_{linear} \tag{14}$$

P' is the non-linearity of pressure. The * sign indicates that pressures are normalized with the outlet pressure. Non-linearity pressure in Lattice Boltzmann Method applications is compared with analytical results.

In this investigation effects of boundary conditions with wide range Knudsen numbers (0.005, 0.01, 0.05, 0.1, 0.15) are studied for different pressure ratios (1.5, 2, 2.5) and mesh numbers (21x2100, 42x4200) in two dimensional micro channel. At different values of accommodation coefficient $a_c = 0.99$ is the closest to analytical results and $r_f = 0.8$ is best matching value with analytical results within reflection factors that depends on the numerical simulations of LBM. Knudsen number equals 0.01 and mesh sizes are 21 in y direction, 2100 in x direction (Fig. 3). It (Fig. 3) shows that non-linearity of pressure (P') with non-dimensionalized x (X) at different boundary condition and different pressure ratios. Moreover, it shows that analytical results.

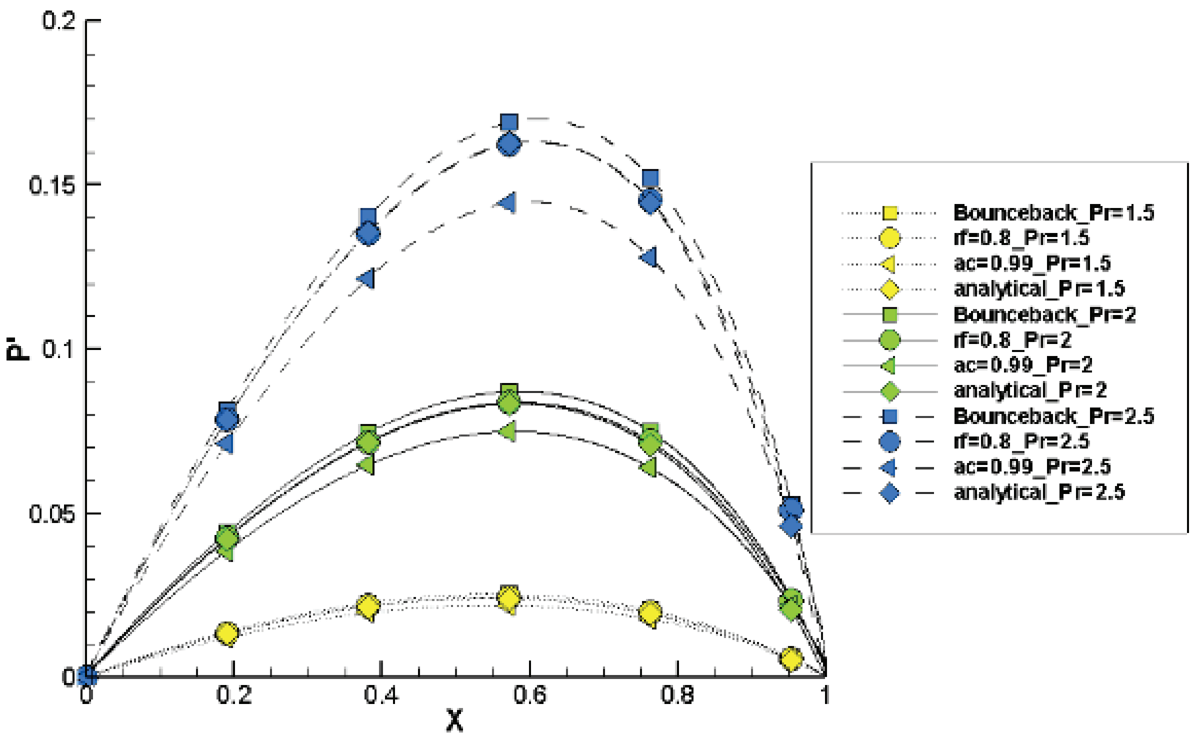

Fig. 3. The effect of boundary conditions at different pressure ratios on the non-linearity of pressure along the channel length (Kn=0.01, Mesh Sizes=21x2100)

With the decreasing of pressure ratio, non-linearity of pressure decreases and all three boundary conditions approach the analytical solutions. In the LBM simulation for 21x2100 mesh sizes, reflection factor boundary condition results are very close to analytical results. There is a big difference between accommodation coefficient boundary conditions results and analytical results at higher pressure ratios. Bounceback boundary conditions predictions do not give as good results as reflection factor boundary conditions.

The results shown on Fig.4 are calculated with the Knudsen number equals 0.01 and mesh sizes 42 in “y” direction and 4200 in “x” direction. The parameters are the same as in Fig. 3.

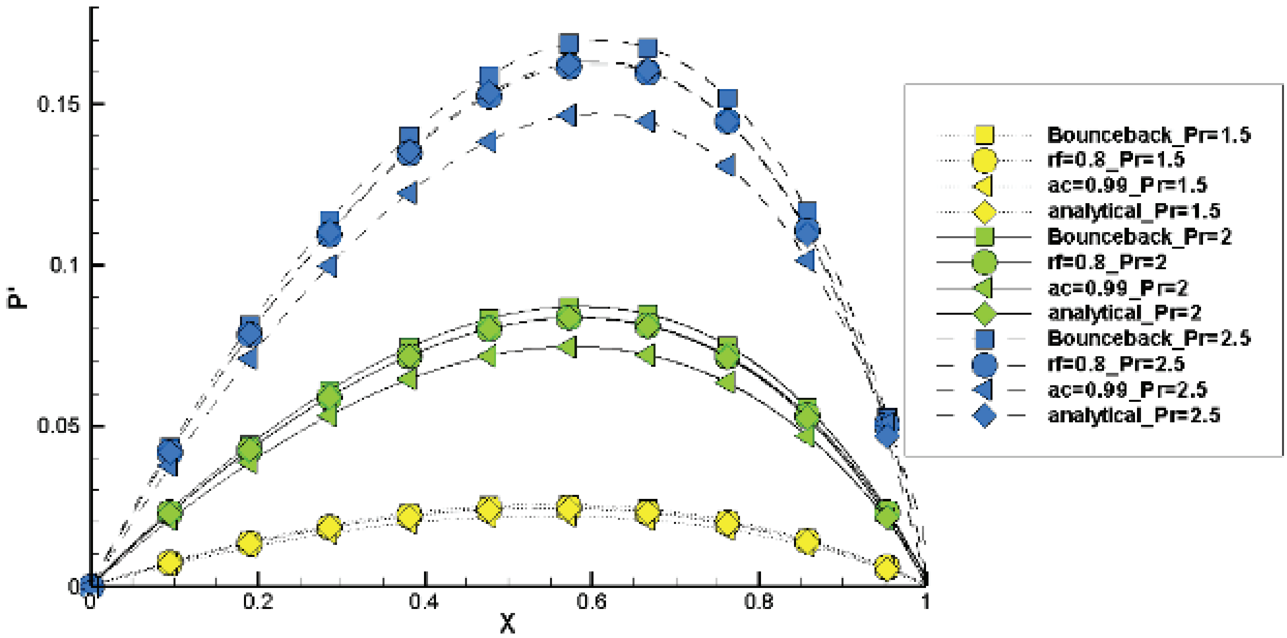

Fig. 4. The effect of boundary conditions at different pressure ratios on the non-linearity of pressure along the channel length (Kn=0.01, Mesh Sizes=42x4200)

Despite the fact that mesh sizes are different from the Fig. 3, reflection factor boundary condition gave good predictions. With the mesh sizes increasing, boundary conditions predictions of non-linearity of pressure have not changed much. Bounce-back boundary conditions for walls is second good boundary conditions in terms of good results. Accommodation coefficient boundary conditions gave good results at lower pressure ratio but with the pressure ratio increasing, predictions recede from analytical results.

CONCLUSION

In the study, a code was written with Lattice Boltzmann Method (LBM) using the Fortran programming language to model different boundary conditions at the wall in the micro channels. LBM simulations show that $r_f = 0.8$ is the best value for reflection factor boundary condition and $a_c = 0.99$ is the best value for accommodation coefficient. Bounce-back boundary condition predictions have little deviations but they show good agreement to the analytical results. Reflection factor boundary condition prediction of non-linearity of pressure is always closer to the analytical values than bounce-back and accommodation coefficient boundary condition predictions. Mesh of micro channel has been increased in order to reach more precise results. But reflection factor boundary condition predictions are closest to analytical results despite the fact that the mesh sizes are different. Because the accommodation coefficient boundary condition value is close to 1, it shows almost diffuse reflection boundary condition. The comparison of the two different mesh sizes shows that 21x2100 mesh sizes are enough for numerical simulations. LBM simulations indicate that numerical results at high Knudsen number flows are in good agreement with analytical results.

 Copyrights© 2017 ISBN 978-954-712-733-3 (Print)

REFERENCES

Koester, D. A., Markus, K. W. & Walters, M. D., (1996). Computer, 29, p.93.

Robinson, E. Y., Helvajian, H. & Janson, S. W., (1995). Aerospace Am., 33. p.9.

Gad-el Hak, M., (1990). The fluid mechanics of microdevices - The freeman scholar lecture. ASME Journal of Fluids Engineering, 121(403), pp. 5-33.

Beskok, A., Karniadakis, G. E., & Trimmer, W., (1996). Rarefaction and compressibility effects in gasmicroflows, Transactions of the ASME, 118, pp. 448-456.

Ho, C. M., & Tai, Y. C., (1998). Micro-electro-mechanical-systems (MEMS) and fluid flows, Ann. Rev. Fluid Mech. 30:579

Tang, G. H., Tao, W. Q., & He, Y. L., (2004). "Lattice Boltzmann method for simulating gas flow in microchannels," Int. J. Mod. Phys. C 15, p.335

Bird, G. A., (1994). Molecular Gas Dynamics and the Direct Simulation of Gas Flows (Oxford University Press, New York)

Chen, S., & Doolen, G. D., (1998). Lattice Boltzmann method for fluid flows, Ann. Rev. Fluid Mech. 30:329

Bhatnagar, P. L., Gross, E. P. & Krook, M., (1954). "A Model for Collision Processes in Gases. I., Small Amplitude Processes in Charged and Neutral One-Component Systems", Physical Review 94, pp.511–525

Qian, Y., d'Humieres, D. & Lallemand, P., (1992). Lattice BGK model for Navier-Stokes equation, Europhysics Letters, 17 (6), pp.479-484

Nie, X., Doolen, G.D. & Chen, S., (2002). Lattice-Boltzmann simulations of fluid flows in MEMS, Journal of Statistical Physics, 107 (1-2), pp.279-289.

Arkilic, E.B., Schmidt, M.A. & Breuer, K.S., (1997). Gaseous slip flow in long microchannels, Journal of Microelectromechanical Systems, 6 (2), pp.167-178